## REMARKS

INTRODUCTION:

In accordance with the foregoing, claims 1, 21, 25, 30, and 35 have been amended. No new matter is being presented, and approval and entry are respectfully requested.

Claims 1-12, 21-33, and 35-41 are under consideration. Claims13-20 are withdrawn. Reconsideration is respectfully requested.

REJECTION UNDER 35 U.S.C. §112:

A. In the Office Action, at page 2, numbered paragraph 3, claims 1, 21, 25, 30, and 35 were rejected under 35 U.S.C. §112, first paragraph, for the reasons set forth therein. This rejection is traversed and reconsideration is requested.

It is respectfully submitted that there may be a misunderstanding of the terminology "fluorene." "Fluorene" is not a misspelling of the term "fluorine," which is a halogen. That is, fluorene has no relation to fluorine (the halogen atom) even though both words are pronounced the same. Fluorene is one of a group of chemicals called polycyclic aromatic hydrocarbons, PAHs for short. Fluorene may generally be represented as follows, wherein C-H bonds are indicated by dotted lines:
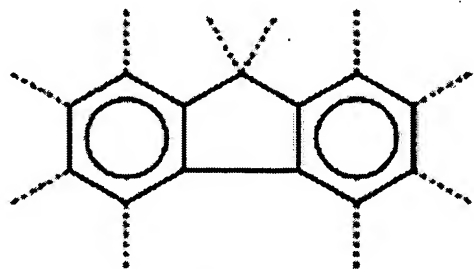

Fluorene

Enclosed herewith, for the Examiner's convenience, are two references which illustrate that "fluorene" does not indicate "fluorine": The Interpretation of the Short Range Disorder in the Fluorene-TCNE Crystal Structure, Int. J. Mol. Sci. 2004, 5, 93-100 and Nist Special Publication 922, Polycyclic Aromatic Hydrocarbon Structure Index, located at http://ois.nist.gov/pah/sp922_detail.cfm?ID=26.

Thus, it is respectfully submitted that, upon review of the meaning of "fluorene," it should be clear that Formula 1, page 4 of the specification, clearly recites a fluorene compound.

It should also be noted that, as recited, in part, in the amended independent claims (also, see, for example, page 4 and 5 of the specification):

"wherein the charge generating layer is formed by coating a charge generating layer

forming composition comprising a fluorene compound represented by Formula 1,

a charge generating material, a binder resin and an organic solvent on the charge

transport layer, and drying:

Formula 1
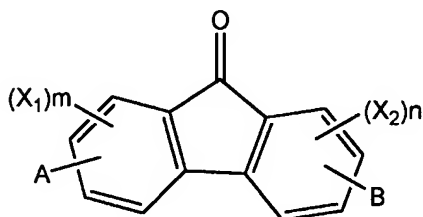
wherein A ~~and B are independently~~ is selected from the group consisting of a carboxyl

group, a substituted or unsubstituted C_2-C_{10} alkoxycarbonyl group and a substituted or

unsubstituted C_2-C_{10} alkylaminocarbonyl group, B is a carboxyl group, X_1 and X_2 are

independently a halogen atom, and m and n are independently an integer from 0 to 3",

the terminology "halogen" is utilized. Halogens are defined to include "fluorine."

Hence, it is respectfully submitted that the specification reasonably provides enablement

for the fluorene and enables any person skilled in the art to which the invention pertains, or with

which it is most nearly connected, to make the substituted fluorene and the invention

commensurate in scope with the claims.

Thus, claims 1, 21, 25, 30, and 35 are submitted to be in allowable form under

35 U.S.C. §112, first paragraph.

B. In the Office Action, at page 2, numbered paragraph 5, claims 2, 22, 26, and 36 were

rejected under 35 U.S.C. §112, second paragraph, for the reasons set forth therein. This

rejection is traversed and reconsideration is requested.

It is respectfully submitted that, as is clear from the description above, as noted in claims

2, 22, 26, and 36 of the present invention, the fluorene molecule of Formula 1 of the present

invention has a carbonyl group (i.e., has an O double-bonded to a carbon in place of two

hydrogens) at the ninth carbon, and the fluorene molecule of Formula 2 has a carbonyl group

(i.e., has an O bond in place of two hydrogens) at the ninth carbon and a carboxyl group coupled

to the fourth carbon.

It is submitted that the above substitutions to the fluorene molecule are clear to one

skilled in the art. Thus, it is submitted that claims 2, 22, 26, and 36 are definite and are in

allowable form under 35 U.S.C. §112, second paragraph.

REJECTION UNDER 35 U.S.C. §103:

In the Office Action, at page 3, numbered paragraph 6, claims 1-12, 21-33 and 35-41 were rejected under 35 U.S.C. §103(a) as being unpatentable over Akasaki et al (USPN 5,153,085; hereafter, Akasaki) in view of Lin et al. (USPN 6,656,650; hereafter, Lin) and Japan Patents 02-097961 and 9-319128. The reasons for the rejection are set forth in the Office Action and therefore not repeated. The rejection is traversed and reconsideration is requested.

Independent claims 1, 21, 25, 30 and 35 have been amended to recite, in part: "wherein the charge generating layer is formed by coating a charge generating layer forming composition comprising a fluorene compound represented by Formula 1, a charge generating material, a binder resin and an organic solvent on the charge transport layer, and drying:

Formula 1
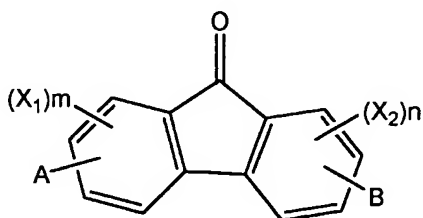
wherein A and B are independently is selected from the group consisting of a carboxyl group, a substituted or unsubstituted C_2-C_{10} alkoxycarbonyl group and a substituted or unsubstituted C_2-C_{10} alkylaminocarbonyl group, B is a carboxyl group, X_1 and X_2 are independently a halogen atom, and m and n are independently an integer from 0 to 3."

It should be noted that It is known that organic compounds are compounds in which elements mainly attached to carbon structures combine, and due to various combinations, a large number of compounds having various characteristics are formed. Even if two compounds differ only by one carbon, the characteristics may be very different. As for isomers, even though the molecular formula is the same, the characteristics of the isomers may be different.

In addition, even when similar combinations of elements are used, the results may be very different. The following description (from http://www.ideafinder.com/history/inventions /story074.htm), which is known to those skilled in the art, shows how difficult it is to utilize combinations of elements to obtain desired results:

> In the period from 1878 to 1880 Edison and his associates worked on at least three thousand different theories to develop an efficient incandescent lamp. Incandescent lamps make light by using electricity to heat a thin strip of material (called a filament) until it gets hot enough to glow. Many inventors had tried to perfect incandescent lamps to "sub-divide" electric light or make it smaller and weaker than it was in the existing arc lamps, which were too bright to be used for small spaces such as the rooms of a house.

Edison's lamp would consist of a filament housed in a glass vacuum bulb. He had his own glass blowing shed where the fragile bulbs were carefully crafted for his experiments. Edison was trying to come up with a high resistance system that would require far less electrical power than was used for the arc lamps. This could eventually mean small electric lights suitable for home use.

By January 1879, at his laboratory in Menlo Park, New Jersey, Edison had built his first high resistance, incandescent electric light. It worked by passing electricity through a thin platinum filament in the glass vacuum bulb, which delayed the filament from melting. Still, the lamp only burned for a few short hours. In order to improve the bulb, Edison needed all the persistence he had learned years before in his basement laboratory. He tested thousands and thousands of other materials to use for the filament. He even thought about using tungsten, which is the metal used for light bulb filaments now, but he couldn't work with it given the tools available at that time.

One day, Edison was sitting in his laboratory absent-mindedly rolling a piece of compressed carbon between his fingers. He began carbonizing materials to be used for the filament. He tested the carbonized filaments of every plant imaginable, including baywood, boxwood, hickory, cedar, flax, and bamboo. He even contacted biologists who sent him plant fibers from places in the tropics. Edison acknowledged that the work was tedious and very demanding, especially on his workers helping with the experiments. He always recognized the importance of hard work and determination. "Before I got through," he recalled, "I tested no fewer than 6,000 vegetable growths, and ransacked the world for the most suitable filament material."

Edison decided to try a carbonized cotton thread filament. When voltage was applied to the completed bulb, it began to radiate a soft orange glow. Just about fifteen hours later, the filament finally burned out. Further experimentation produced filaments that could burn longer and longer with each test. By the end of 1880, he had produced a 16-watt bulb that could last for 1500 hours and he began to market his new invention.

Although Akasaki recites an electrophotographic photosensitive member and image forming apparatus, Akasaki fails to recite a fluorene having a carboxyl group attached thereto, as is recited in amended independent claims 1, 21, 25, 30 and 35 of the present invention. Hence, Akasaki fails to recite the composition of the present invention.

Although Lin recites a member comprising a supporting layer and a photoconductive insulating layer comprising a photogenerating component, a polytetrafluroethylene charge transport particles from about 0.1 microns to about 20 microns component, an electron transport, and a binder, Lin fails to recite a fluorene having a carboxyl group attached thereto, as is recited in amended independent claims 1, 21, 25, 30 and 35 of the present invention.

Although JP 02-097961 recites an electrophotographic sensitive body and image forming method, JP 02-097961 fails to recite a fluorene having a carboxyl group attached thereto, as is recited in amended independent claims 1, 21, 25, 30 and 35 of the present invention.

Although JP09-319128 recites an electrophotographic photoreceptor having a charge generating layer and a charge transfer layer containing a hole transfer material on a conductive substrate, wherein a base layer containing a fluorene compound is formed between the

conductive substrate and the charge generating layer or in the electrophotographic photoreceptor produced by laminating a charge generating layer and a charge transfer layer on a conductive substrate, the charge generating layer contains at least a charge generating material, a hole transfer material, an electron transfer material and a binder resin, and a fluorene compound used as the electron transfer material, JP09-319128 fails to recite a fluorene having a carboxyl group attached thereto, as is recited in amended independent claims 1, 21, 25, 30 and 35 of the present invention.

As noted above, different compounds tend to react differently, sometimes due to a tertiary structure which may result from a presence of different chemical element(s). Hence, it is respectfully submitted that none of Akasaki et al (USPN 5,153,085), Lin et al. (USPN 6,656,650), JP02-097961 and/or JP09-319128, alone or in combination, recite or suggest the present claimed invention.

Thus, is it submitted that amended claims 1, 21, 25, 30, and 35 are patentable under 35 U.S.C. §103(a) over Akasaki et al (USPN 5,153,085) in view of Lin et al. (USPN 6,656,650) and Japan Patents 02-097961 and 9-319128. Since claims 2-12, 22-24, 26-29, 31-33 and 36-41 depend from amended independent claims 1, 21, 25, 30, and 35, claims 2-12, 22-24, 26-29, 31-33 and 36-41 are submitted to be patentable under 35 U.S.C. §103(a) over Akasaki et al (USPN 5,153,085) in view of Lin et al. (USPN 6,656,650) and Japan Patents 02-097961 and 9-319128 for at least the reasons that amended independent claims 1, 21, 25, 30 and 35 are submitted to be patentable under 35 U.S.C. §103(a) over Akasaki et al (USPN 5,153,085) in view of Lin et al. (USPN 6,656,650) and Japan Patents 02-097961 and 9-319128.

CONCLUSION:

In accordance with the foregoing, it is respectfully submitted that all outstanding objections and rejections have been overcome and/or rendered moot, and further, that all pending claims patentably distinguish over the prior art. Thus, there being no further outstanding objections or rejections, the application is submitted as being in condition for allowance which action is earnestly solicited.
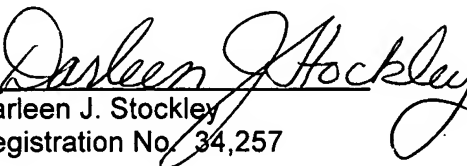
If the Examiner has any remaining issues to be addressed, it is believed that prosecution can be expedited by the Examiner contacting the undersigned attorney for a telephone interview to discuss resolution of such issues.

If there are any underpayments or overpayments of fees associated with the filing of this Amendment, please charge and/or credit the same to our Deposit Account No. 19-3935.

Respectfully submitted,

STAAS & HALSEY LLP

Date: _December 7, 2005_   By: _____
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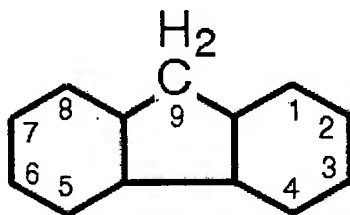Telephone: (202) 434-1500
Facsimile: (202) 434-1501

Polycyclic Aromatic Hydrocarbon Structure Index
Lane C. Sander and Stephen A. Wise

Number	Name
11	**Fluorene**

o-Biphenylenemethane
Diphenylenemethane
9H-Fluorene
2,2'-Methylenebiphenyl
2,3-Benzidene
o-Biphenylmethane

CAS:	86-73-7	**MW:**	166	**L/B:**	1.520
Width:	7.521	**Length:**	11.431	**Thickness:**	4.241

Appears on Page: 2 (View page)

Download editable structure file: Molecule (.mol) | Windows metafile (.wmf)

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ECCC9

The Interpretation of the Short Range Disorder in the Fluorene-TCNE Crystal Structure

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Abstract: The interpretation of the short-range static and/or dynamic disorder in a crystal structure from X-ray data is often a rather complex problem. Recently, we synthesized and characterized three co-crystalline complexes between fluorene, showing C_{2v} symmetry, and three electron withdrawing D_{2h} compounds, employing FTIR and Raman spectroscopy and single crystal X-ray diffraction techniques. The crystal structures of the complexes of fluorene with the three different electron withdrawing molecules are disordered in the solid state and only approximate structures were obtained by refinement of the single crystal data. Indeed, the fluorene moiety presents a very irregular geometry, showing for example C-C bonds ranging from 1.25Å to 1.75Å. Graphical inspection of the solved crystal structures indicates that the fluorene molecules in these co-crystalline complexes can assume two possible positions, both with 50% population. A two-step procedure to improve the disordered models is described. At first, the two possible ordered structures, with the fluorene molecule in only one of the two populated positions, are "separated" by molecular graphic techniques and then their geometry is fully optimized employing the periodic *ab initio* "CRYSTAL" code to obtain a chemically sensible model with reasonable distances and angles. The main aim of this communication is to demonstrate that ordered models can be obtained, starting from a disordered crystal structure, focusing our attention on the fluorene-TCNE molecular complex.

Keywords: disordered crystal structures, molecular crystals, *ab initio* periodic calculations.


Introduction

Short-range static and/or dynamic disorder is an "undesirable guest", which affects a considerable number of crystal structures. When some disorder is found in a crystal structure, it is often impossible to obtain sensible geometric features such as bond distance and angles, intermolecular contacts and packing arrangements. Theoretical calculations can then be used to achieve a better interpretation of the electron density from a crystal structure presenting various degrees of structural short-range disorder.

Recently, we decided to study the possibility of co-crystallizing the fluorene molecule, which presents a C_{2v} symmetry, with an electron withdrawing molecular unit of higher symmetry, in order to obtain a charge transfer (CT) complex. We have chosen the fluorene molecule because it is well known for its optical responses and, for these properties, its use is investigated in active optically designed materials [1-3]. We employed, as fluorene counterparts, tetracyanoethylene (TCNE in Figure 1), 1,2,4,5 tetracyanobenzene (TCNB) and 7,7,8,8-tetracyanoquinodimethane (TCNQ), all presenting D_{2h} symmetry. We were aware that the crystal structures of fluorene containing molecular complexes were disordered [4-7].

The three complexes have been characterized employing spectroscopic techniques (FTIR and Raman spectroscopy) and single crystal X-ray diffraction analysis. The analysis of the X-ray diffraction data was complicated by the difficulty in assigning the correct space group, because of the uncertainty on the presence or not of an inversion center and the possible disorder of the fluorene unit. Therefore some *ab initio* periodic theoretical calculations have been performed, in order to solve the problem inherent to the interpretation of the crystal data. All the experimental results, together with the synthesis and the crystallization techniques, will be fully described in a separated paper [8]. The aim of this paper is to show that sensible models of the crystal structures can be obtained by a two step procedure: (i) the disordered experimental structure is first separated into its components by graphical manipulation; (ii) then the geometry is optimized by means of *ab initio* quantum-chemical calculations, carried out with the CRYSTAL code [9]. The Hartree-Fock (HF) level of theory was adopted within the LCAO approximation and periodic boundary conditions. Recently, thanks to the implementation in CRYSTAL [9] of the analytical HF nuclear gradient [10,11], geometry optimization

Fluorene   TCNE
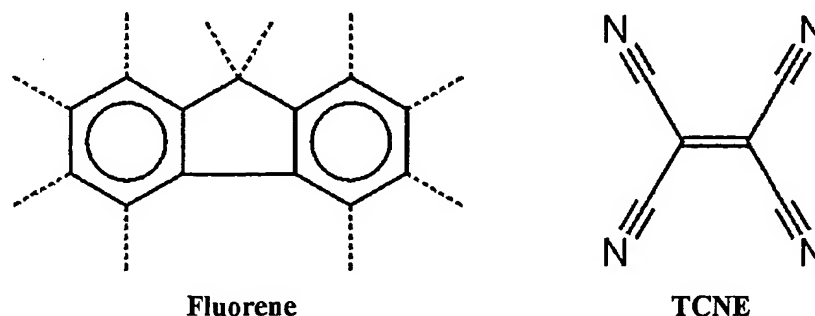
Figure 1. Fluorene and its D_{2h} counterpart in the co-crystalline complex (C-H bonds are indicated by dotted lines).

of periodic systems has become feasible in routine calculations [12]. Thus crystal structures can be optimized and an *ab initio* quantum mechanical structure refinement can be performed. In particular, here we report in details the above-described procedure, applied to the structure of the Fluorene/Tetracyanoethylene complex (hereafter named complex **1**).

Computational Details

All calculations have been performed by using the CRYSTAL code [9]. A fixed-cell unconstrained optimization of the atomic coordinates is performed by fixing the cell parameters to the values obtained from the X-ray diffraction experiments. The forces acting on the atoms are obtained by using the recent implementation in CRYSTAL of analytical HF gradients [10], and used to relax the atom positions towards equilibrium using a modified conjugate gradient algorithm as proposed by Schlegel [13]. Standard Pople 3-21G, 6-21G, 6-21G(d) and 6-21G(d,p) basis sets [14] were employed to obtain the optimized geometries and to compute the corresponding lattice energy (L.E.), employing the following relation:

$$\text{L.E.} = E(X)_{CRYSTAL} - E(Fluorene)_{MOLECULE} - E(TCNE)_{MOLECULE} \qquad (1)$$

where X can be complex **1a** or **1b**.

Default tolerances for the integral calculations (except for T5 = 14) [9] and geometry optimization [12] were adopted. The number of reciprocal lattice points (k-points) at which the Hamiltonian matrix has been diagonalized is 36, corresponding to a shrinking factor S=4 [9].

Results

From a Disordered Crystal Structure to an Ordered Model

The crystal structure of complex **1** is disordered in the solid state and only an approximate structure can be obtained by refinement of the single crystal data. Fluorene (the electron donating C_{2v} molecule) always presents a very irregular geometry, showing for example C-C bonds ranging from 1.25Å to 1.75Å. Conversely, the electron withdrawing D_{2h} molecules (i.e. the counter part of fluorene in the complexes) are ordered, thanks to their higher symmetry as already described by Muhle et al. [5]. Graphical inspection of the crystal structures suggests that the fluorene molecules in these co-crystalline complexes can assume two possible positions (indicated by black and white bonds in Figure 2), related by an inversion center, both with 50% population.

Molecular manipulations by means of the MOLDRAW [15] and XP [16] programs were performed to generate the two possible models with the two ordered positions of the fluorene molecule without modifying the crystallographic periodicity. This artificial graphical separation process is illustrated in Figure 2 for complex **1**. The model crystal structure with the combination of the fluorene molecule
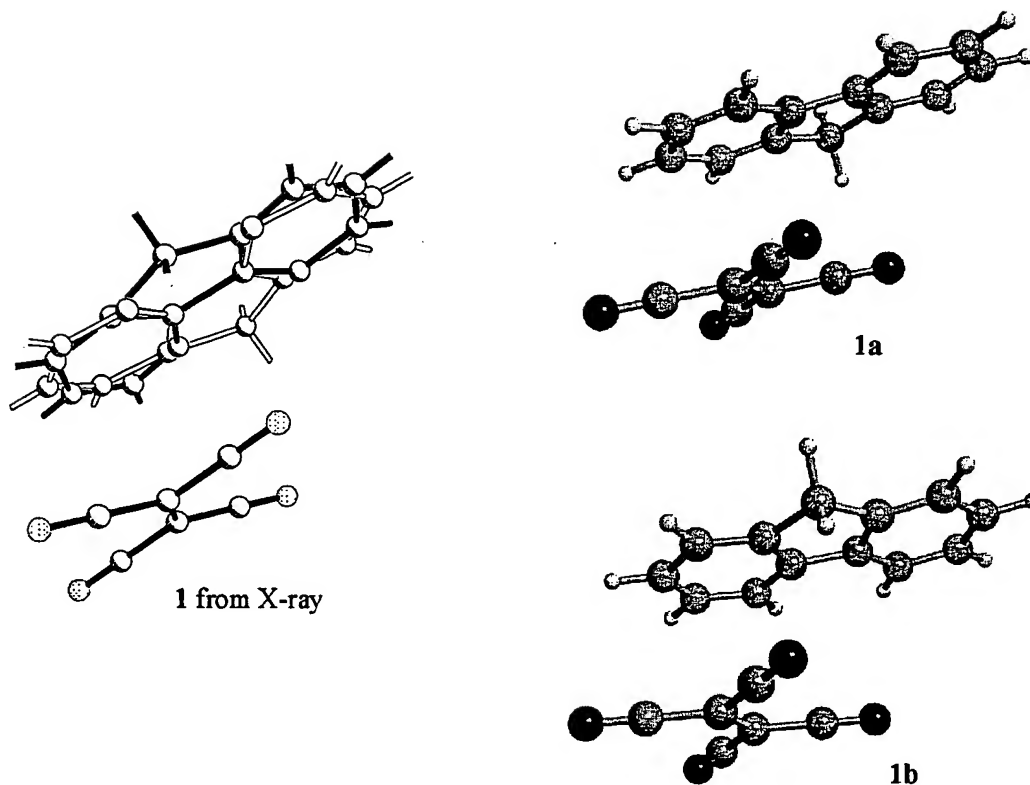
Figure 2. Sketch of the graphical separation process used to obtain the two distinct ordered structures from the disordered crystal structure of **1**, where the black and white bonds indicate the **1a** and **1b** positions respectively.

labeled **a** with its TCNE counterpart is named **1a**, and that with the combination of molecule **b** with its TCNE counterpart is named **1b**. Of course, the model ordered structures **1a** and **1b**, derived from the centrosymmetric P-1 X-ray structure, belong to the related non-centrosymmetric space group P1. Starting from these model structures their full geometry optimization was performed to obtain sensible geometries and to verify whether the **a** and **b** positions present the same stability. Besides, an estimate of the lattice energy (L.E.) was obtained by subtracting the gas phase energy of the isolated molecules from the crystal energy, according to eq. 1.

Geometry Optimization

In this paragraph we describe the geometric features of compounds **1a** and **1b** after geometry optimization of the model structures (Figure 2) at the HF level, employing increasingly larger basis sets.

No significant changes in the values of bond distances and angles can be observed passing from the HF/3-21G to the HF/6-21G(d,p) level of theory and therefore only the results obtained at the HF/6-

21G(d,p) level are reported.

The more dramatic changes between the X-ray structure and that after geometry optimization involve the 5-member ring of fluorene, shown in Figure 3 with the adopted labeling scheme. Figure 3 and Table 1 show the comparison between the geometrical features of the 5-member ring before and after full geometry optimization of 1a. It can be seen that the geometry optimization gives a chemically sensible model with the expected bond lengths and angles, starting from the rather deformed geometry obtained from the X-ray data. Indeed the optimized bond distances and angles (see Figure 3 and Table 1) are rather similar to those from the X-ray crystal structure of fluorene alone [17], which is not disordered. The comparison between the geometry of fluorene alone in the crystal structure [17] and of fluorene after HF/6-21G(d,p) full geometry optimization suggests that this level of theory is sufficiently accurate to describe the geometry of fluorene itself. Therefore the discrepancies between the calculated and experimental geometries of fluorene in complex 1 are certainly due to the structural disorder of the X-ray structure of complex 1.
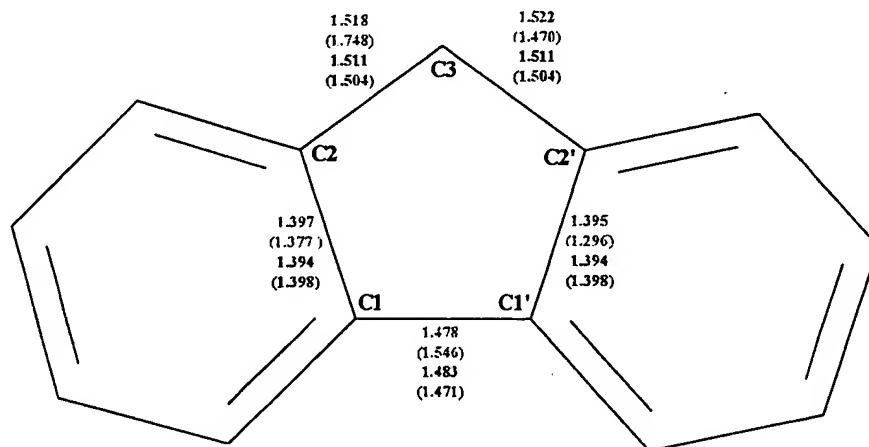

Figure 3. The 5-member ring of fluorene and its labeling. The values after geometry optimization are compared with the corresponding values from the X-ray data refinements (in parenthesis) of 1a (in red) and of fluorene alone [17] (in blue).

Table 1. Bond angles of the 5-member ring of fluorene in 1a fluorene alone [17] from the X-ray data and after full geometry optimisation.

Angle [°]	1a 6-21G(d,p)	1a X-ray	Fluorene[$] 6-21G(d,p)	Fluorene[*] X-ray
C1-C2-C3	110.3	102.4	110.4	110.4
C2-C3-C2'	102.2	120.0	102.5	102.7
C3-C2'-C1'	110.5	102.3	110.5	110.4
C2'-C1'-C1	108.4	107.2	108.3	108.3
C1'-C1-C2	108.5	128.3	108.7	108.3

($) After HF/6-21G(d,p) periodic full geometry optimisation of the geometry from ref [17];
(*) From reference [17].

In Figure 4 the crystal packing of the complex **1a**, after geometry optimization at the HF/6-21G(d,p) level, is shown. The intermolecular interactions driving the crystal packing are:

- the weak C-H·····N interactions between molecules on the same plane (dotted lines in Figure 4), with H·····N distances in the range 2.55-2.91 Å;

- the stacking interactions between the fluorene and TCNE molecules on adjacent parallel planes. The distance between the centers of the C=C bond in TCNE and of the facing phenyl group in fluorene (the two moieties, involved in the CT, shown in Figure 4), is about 3.31Å. This value is very close to the inter-planar distance (~3.28Å), indicating an almost perfect facing between TCNE and the phenyl group in fluorene.

It is worth noting that the intermolecular distances obtained from the disordered crystal structures were too crude to allow a reliable discussion of the above packing geometry.
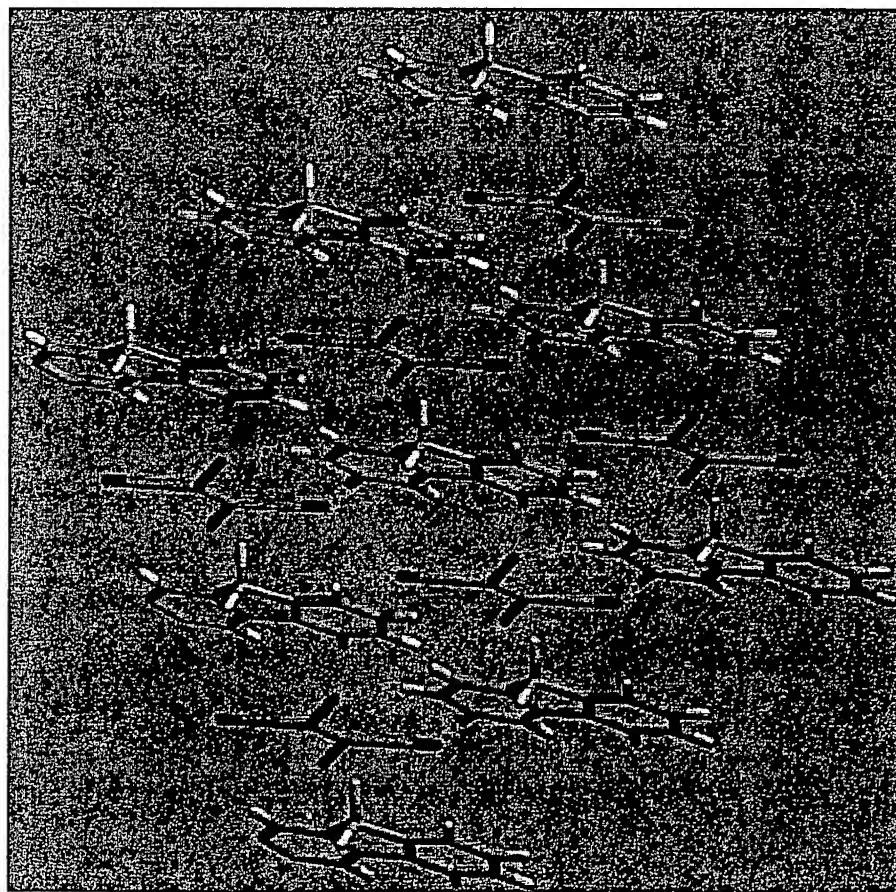

Figure 4. The crystal packing arrangement of compound **1a** after geometry optimization.

Energy Results

In Table 2 the energetic features of the studied models after full geometry optimization are reported. The optimized structures **1a** and **1b** retain an enantiomeric relation and have very similar total energy values after geometry optimization. Indeed the two fluorene dispositions differ by less than 0.2 kJ/mol at the HF/6-21G(d,p) level of theory and therefore can be considered equivalent. The presence of the inversion center (relating the two equivalent fluorene positions in the actual disordered crystal structure) is then explained and confirmed.

As already mentioned, the described procedure also allows an approximate estimate of the lattice energy (see eq. 1). For instance the value calculated for **1** at the HF/3-21G level is: L.E. =136.2 kJ/mol. The comparison of the values obtained for different complexes can be correlated with the experimental spectroscopic evidences on the weak interactions holding together the complexes in the solid state and in solution (a detailed comparison will be reported in a separated paper [8]).

Table 2. Total energy for the two model structures of compound **1** (data in Hartrees, 1 Hartree = 2625.5 kJ/mol) and relative stability $\Delta E = E_{1a}-E_{1b}$ (in kJ/mol) at different levels of calculation.

	1a	**1b**	**ΔE**
HF/3-21G	-937.7946535	-937.7941936	-1.21
HF/6-21G	-942.0021077	-942.0021458	0.10
HF/6-21G(d)	-942.4568083	-942.45694895	0.37
HF/6-21G(d,p)	-942.4857835	-942.4858601	0.20

Conclusions

In this work the CRYSTAL code was employed to elucidate the disordered crystal structure, obtained from X-ray single crystal analysis on a molecular complex of fluorene with the electron withdrawing TCNE molecule (Figure 1). The crystal structure analysis of complex **1** (Figure 2 left) indicated that the fluorene molecule is disordered over two symmetry related positions (**1a** and **1b** in Figure 2 right) in the centrosymmetric *P-1* crystal structure. *Ab initio* periodic calculations on the two graphically separated non-centrosymmetric *P1* model crystal structures indicated that these two positions are equivalent from the geometric and the energetic point of view. The presence of an inversion center is thus explained and confirmed and the correctness of the X-ray data refinement in the *P-1* space group is verified. The geometry of the disordered fluorene obtained in this way is poorly defined and only by the *ab initio* full geometry optimization of the *P1* model structures could a sensible fluorene moiety, with the expected bond distances (Figure 3) and angles (Table 1) and intermolecular contacts (Figure 4), be obtained, together with an estimate of the lattice energy.

The main scope of the present paper is to show that the deformed geometry obtained from the X-ray analysis of a disordered crystal structure can be improved by the use of the new features of the

CRYSTAL code, which allow the *ab initio* full geometry optimization of a periodic structure. A full account of the crystallographic and theoretical implications of the described procedure will be given elsewhere. [18].

Acknowledgements

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